

X-RAY PHOTOELECTRON SPECTROSCOPY INTERFACE STUDIES

The JPL surface chemistry laboratory measured the detailed chemical environment of the silicon/silicon dioxide (Si/SiO_2) interface using X-ray photoelectron spectroscopy (XPS) and related these measurements to the reliability and radiation hardness of microelectronic devices.

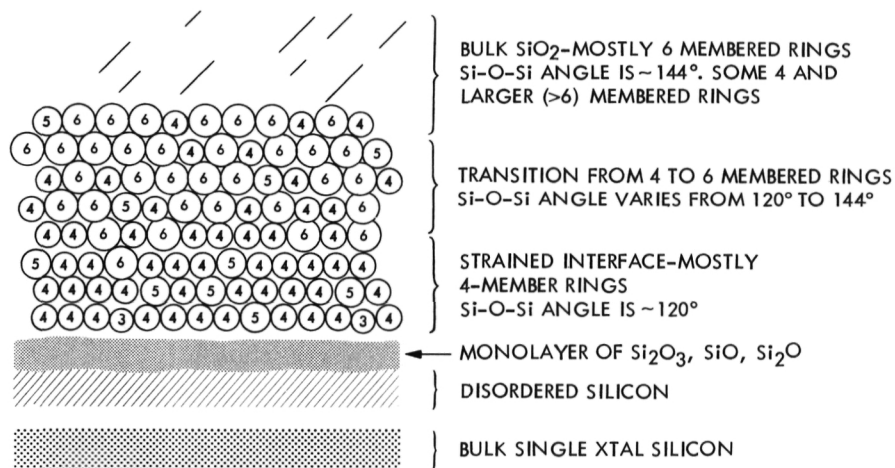
Using XPS and chemical depth-profiling techniques, it was found that the oxide is SiO_2 to within one monolayer of the silicon substrate. An abrupt chemical interface (approximately one monolayer) was found with a mixed composition comprising Si_2O_3 , SiO , and Si_2O . Except at this interface, the SiO_2 chemical units are arranged in ring structures whose average size depends upon distance from the interface. The bulk of the oxide is composed of 6-membered rings similar to alpha-quartz. Within 30 angstroms of the interface, there is a strained layer of 4-membered rings induced by the lattice mismatch between the bulk oxide and the substrate. This layer's composition is dependent upon the details of the wafer processing chemistry.

The ring model is illustrated schematically in the top left figure, where circles are used to indicate network rings. This observed structure has been used to develop a structural model for hole and electron trap generation by ionizing radiation. These traps have been observed during *in situ* experiments examining the interfacial regions of radiation-hard and -soft gate oxides.

XPS techniques have also been extended to the investigation of metal/semiconductor interfaces. The primary goal of these studies has been to examine these interfacial regions nondestructively and to relate the observed chemical structure to such electrical properties as Schottky-barrier heights and ohmic contact formation. One experimental approach is to deposit

sequential monolayers of a metal on silicon under ultra-high vacuum conditions. By simultaneously monitoring the metal and silicon photoemission signals as a function of metal coverage, the chemical development of the interface has been followed *in situ*.

These metal/silicide/silicon interfaces have also been investigated by studying the metal and silicon XPS signals during *in situ* growth of the metal silicide. The experiments are yielding information on such fundamental questions as the variation of structure and chemical bonding across the interfacial region.



Schematic model of the Si/SiO_2 interface as determined using x-ray photoelectron spectroscopy.

Figure (opposite page): 3-D plot of the $\text{Ni}2p$ core levels illustrating the intensity change and chemical shift observed during sequential silicide compound formation.

